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Application and Implementation of the ParFlow Groundwater Flow Model

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The ParFlow model is being designed and developed to rapidly simulate saturated groundwater flow and chemical migration processes in large-scale, three-dimensional geologic formations. By "large-scale", we refer to application problems that are both large in their spatial extent and detailed with respect to spatial resolution. These conditions are often generated by the need to understand the impacts of small-scale geologic heterogeneity (on the order of 1 to 10 m) on the rates of groundwater flow and patterns of tracer or chemical migration that evolve over much larger scales (say between 100 to 1000 m, or more). The relevant computational problems can often exceed millions or tens of millions of unknowns.

The interest and detail in this type of problem has largely been motivated by nationwide efforts to assess and remedy groundwater quality problems associated with industrial or defense complex contamination, long term agricultural practices, and broader groundwater resource management issues. In this context, groundwater simulations are typically used to provide a rational basis for analyzing issues related to long-term health risks, natural attenuation behavior, the cost-effectiveness of contamination remediation technologies, and so forth.

Historically, oversimplified conceptualizations of system behavior have been used as the basis for many types of design and modeling studies. The role of geologic heterogeneity has not been

frequently considered, even though its impact in many instances is becoming increasingly apparent and relevant. Although simplified approaches are usually justified in some sense by the lack of sufficient characteristic geologic data (to fully specify the distribution of heterogeneous properties, for example), they do nothing to scientifically address or quantify the uncertainties implied by the paucity and variability of information usually available. This can lead to unreliable and over-engineered remedial solutions that are unnecessarily expensive. Practical techniques for dealing with the important effects of heterogeneity in geologic systems are few and far between.

Our approach for "dealing" with heterogeneity involves the use of ParFlow to enable large-scale, highly-resolved simulations of flow, transport and reaction phenomena in systems that recreate the character and detail of physical and chemical variability observed in natural physical formations. This is achieved through the use of multiple, equally likely stochastic "realizations" of the system heterogeneity within known, or deterministic, structural boundaries of a formation. It is meant to complement and bridge the gap between theoretical (e.g., stochastic) models and various laboratory and field experimental studies focused on discerning the important features and impacts of heterogeneity.

ParFlow has been developed for use on a variety of computational platforms, ranging from large-scale, massively parallel computers such as the Cray T3D, to smaller clusters of engineering workstations, to Windows 95 PC's. It has been optimized for repeated large-scale flow simulations by incorporating a concise, hierarchical, and grid-independent representation of hydrostratigraphic flow units, direct generation of the stochastic property fields via several parallel generation techniques, and an efficient solution of the discretized equations using a multigrid preconditioned conjugate gradient (MGCG) technique.

The use of repeated "Monte Carlo" simulations allows the uncertainty associated with any one stochastic simulation to be quantitatively bracketed by the results of the ensemble. Nevertheless, it reinforces the need to achieve efficiency in any one simulation so that all may be accommodated. To this end, the MGCG technique was developed as the core of the ParFlow flow model. MGCG combines the scalability and speed of multigrid algorithms (i.e., the convergence rate is preserved regardless

of problem size) with the guaranteed convergence properties of conjugate gradient methods.

The entire process of doing multiple realization simulations implies that additional efficiencies with respect to data manipulation be developed. This point is made clear by the fact that importing and exporting millions of property and simulation data values can dominate the wall-clock time of any one simulation. With this in mind, domain, geostatistical, boundary condition, and other conceptual model specifications for a given problem occur in ParFlow through a series of grid-independent inputs. These serve to reduce the volume of input data required for one or more Monte Carlo runs. At run time, a grid resolution is specified, and the requisite interpolation and property assignments onto the grid are done automatically. Moreover, internal routines for the parallel generation of stochastic property fields (currently including a parallel Turning Bands method and a conditional Parallel Gaussian algorithm) are also invoked. In addition, newer features for real-time graphical output and solution interrogation and assessment are also being developed. Although the grid-independent approach was motivated by the need to minimize I/O choke points in large problems, it also allows the early stages of conceptual model development to be unencumbered by concerns related to the grid and its optimal size. Because of ParFlow's portability, much of the time-consuming initial aspects of conceptual model development and testing can now be relegated to smaller computers.

At this time, the transport component of the ParFlow model includes an explicit Godunov advection routine for the simulation of non-dispersive transport of dilute (neutrally buoyant) solutes within the steady groundwater flow regime. This capability is currently complemented by an external serial particle-grid transport model (SLIM). Although the Godunov scheme also forms a basis for multiphase flow components of Parflow now under development, its transport performance is hampered by extreme time-step limitations produced by locally large velocities near wells or in fast flow channels in the formation. These issues will be ameliorated to some extent by the incorporation of temporal sub-cycling technique to localize the small time step calculations in areas where they are required, and also by the inclusion of an internal particle transport model within ParFlow.

During the presentation, several example applications of ParFlow will be shown. These will serve to illustrate ParFlow's computational performance on several test problems and document its application to several field and contaminant remediation sites in California. Additional modifications to ParFlow to improve its practical applicability and future potential applications of this modeling approach will also be discussed.

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